WHAT IS CLAIMED:

1. A method of forming a generated conformation of a molecular system comprising generating a molecular dynamics trajectory of said molecular system, wherein said trajectory is initiated by assigning to each atom in said molecular system a set of initial parameters comprising an initial velocity vector and an initial conformation wherein each atom in said molecular system is disposed in an initial position, and wherein said molecular dynamics trajectory is propagated by a computational procedure comprising:

(a) calculating a current force exerted on each atom (i) by calculating a derivative of an energy function describing interactions between said atom (i) and other atoms in said molecule;

(b) determining a guiding force g_i describing an average along a portion of said trajectory of a force exerted on said atom (i);

(c) determining a current position and velocity of said atom (i) by adjusting said previous position and velocity according to the equation $m_i a_i = f_i$, wherein m_i is the mass of atom (i), a_i is an acceleration of atom (i) and f_i is a force obtained by adding said current force calculated in (a) and said guiding force determined in (b);

(d) replacing said previous position and velocity of said atom (i) with said current position of said atom (i);

(e) repeating steps (a) to (d) for one or more iterations to generate said trajectory;

(f) forming said generated conformation by disposing the atoms of said molecular system in respective current positions obtained during a given iteration; and processing said generated conformation to determine a structural, energetic, thermodynamic or kinetic property of said molecular system.

2. The method of Claim 1, wherein determining said guiding force g_i comprises accumulating a force along a portion of said trajectory to obtain a cumulative force, dividing said cumulative force by the length of said portion of said trajectory to obtain an average cumulative force and multiplying said average cumulative force with a parameter λ to obtain said guiding force g_i, wherein λ is not zero.

3. The method of Claim 2, wherein said portion of said trajectory is defined by a simulation period according to said molecular system.

4. The method of Claim 2, wherein said parameter λ has a value between 0.01 and 5.00.

5. The method of Claim 2, wherein said cumulative force is obtained by adding said current force exerted on said atom (i) calculated in step (a) along said portion of said trajectory.

6. The method of Claim 2, wherein said cumulative force is obtained by determining an external force exerted on said atom (i) obtained by deriving an energy function describing the interactions between said atom (i) and other atoms in said molecular system which are not positioned within three covalent bonds or less from said atom (i).

7. The method of Claim 2, wherein obtaining said cumulative force comprises determining for atom (i) and each atom j positioned within three covalent bonds from said atom (i) an external force exerted on said atom (i) or atom j obtained by deriving an energy function describing the interactions between said atom (i) or atom j and other atoms in said molecule which are not positioned within three covalent bonds or less from said atom (i); for each atom j multiplying said external force with a mass ratio m_i/M_j to obtain a mass weighed external force; and adding to said external force exerted on said atom (i) said mass weighed external force obtained for each atom j to obtain said cumulative force.

8. The method of Claim 1, further comprising scaling the velocities of all atoms of said molecular system so that the total energy remains constant.

9. A method of generating a folded structure of a polypeptide comprising generating a molecular dynamics trajectory according to the method of claim 1, wherein said molecular system comprises said polypeptide and said initial conformation describes said polypeptide in an extended form and said generated conformation describes said polypeptide in a folded form.

10. The method of Claim 9, wherein said folded conformation comprises an alpha helix, a β-hairpin, a β-sheet or a mixture thereof.

11. The method of Claim 9, wherein said polypeptide defines a primary structure of a protein.

12. The method of Claim 11, wherein said polypeptide is a protein of known amino acid sequence and unknown tertiary structure, wherein processing said conformation comprises predicting a tertiary structure of said protein.

13. A method of docking a guest molecule into a host molecule comprising generating a molecular dynamics simulation according to the method of Claim 1, wherein said molecular system comprises said guest and host molecules, and wherein said initial conformation describes said guest molecule positioned outside said host molecule and said molecular dynamics trajectory comprises a generated conformation wherein said guest molecule is positioned within said host molecule.

14. A method of generating a phase transition of a molecular system by the method of Claim 1, wherein said initial conformation describes said molecular system in an initial physical state and said generated conformation describes said system in a physical state different from said initial physical state.

15. The method of Claim 14, wherein said initial physical state describes a liquid and said generated physical state describes a solid phase.

16. A method of generating a molecular dynamics trajectory of a molecular system comprising:

generating a succession of snap shots, each snap shot describing a frame of said molecular system, and each snap shot is separated from a previous snap shot in said trajectory by a time step δt, said trajectory having a total duration of up to $t_{final} = N\delta t$, wherein N is a predetermined integer greater or equal to 1, and wherein said trajectory is initiated by assigning to each atom in said molecular system a set of initial parameters comprising an initial velocity vector and an initial frame wherein each atom in said molecular system is disposed in an initial position;

(a) propagating said molecular dynamics trajectory by a computational procedure comprising for each atom (i):

(1) calculating a current force exerted on said atom (i) by deriving an energy function describing interactions between said atom (i) and other atoms in said molecular system;

(2) determining a guiding force g_i describing an average along a portion of said trajectory of a force exerted on said atom (i);

(3) determining a current position and velocity of said atom (i) by adjusting said previous position and velocity according to the equation $m_i a_i = f_i$, wherein m_i is the mass of atom (i), a_i is an acceleration of atom (i) and f_i is a force obtained by adding said current force calculated in (1) and said guiding force determined in (2);

(4) replacing said previous position and velocity of said atom (i) with said current position and velocity of said atom (i);

(b) repeating step (a) for up to N-1 iterations to generate said trajectory; and processing said trajectory to determine a structural, thermodynamic, kinetic or energetic property of said molecular system.

17. The method of Claim 16, wherein said guiding force g_i is calculated by averaging the force exerted on atom i over all conformations near current conformation.

18. The method of Claim 16, wherein said guiding force g_i is calculated by averaging the force exerted on atom i over previous certain period of time.

19. The method of Claim 16, wherein said guiding force $g_i(t_p)$ is calculated by eq.

$$g_i(t_p) = \frac{i}{L} \sum_{j=P-L}^{P} \left[f_i(t_j) + \lambda g_i(t_j) \right]$$

20. The method of Claim 16, wherein said guiding force $g_i(t_p)$ is calculated by eq.

$$g_i(t_p) = (1 - \frac{1}{L})\, g_i(t_{p-1}) + \frac{1}{L} \left[f_i(t_p) + \lambda g_i(t_{p-1}) \right]$$

21. The method of Claim 16, wherein said guiding force $g_i(t_p)$ at a snap shot $t_p = p\delta t$, wherein p is $\leq N$ is equal to a guiding force $g_i^{(s)}(t_p)$, wherein $g_i^{(s)}(t_p)$ is determined according to equation (1):

$$g_i^{(s)}(t_p) = (1 - 1/L) g_i^{(s)}(t_p - \delta t) + (1/L) m_i \sum_{j \in Si} \{(f_j^{(s)}(t_p) + \lambda g_j^{(s)}(t_p - \delta t))/M_j\}$$

wherein $g_i^{(s)}(t_p)$ is the guiding force exerted on atom (i) at a snapshot t_p, $g_i^{(s)}(t_p - \delta t)$ is the guiding force exerted on atom (i) at a snapshot $(t_p - \delta t)$, L is a length of a portion of said trajectory employed in computing said cumulative guiding force,

m_i and M_j are atomic masses of atoms (i) and j, respectively, S_i is a group formed by all atoms in said molecular system which are linked to atom (i) through three covalent bonds or less, $f_j^{(s)}(t_p)$ is a force exerted on atom j by all atoms in said molecular system which are not in group S_i; λ is a predetermined guiding force multiplication factor.

22. The method of Claim 17, wherein determining a current position $r_i(t_p + \delta t)$ of said atom (i) at snap shot p +1, comprises adjusting a position of said atom according to equation (2):

$$r(t_p + \delta t) = r(t_p) + v_i(t_p + \delta t/2)\delta t$$

wherein $r(t_p)$ is the position of atom (i) at a snap shot immediately preceding the snap shot $t_p + \delta t$ and $v_i(t_p + \delta t/2)$ is the velocity of atom (i) at half a time step δt separating snap shots p and p +1, wherein $v_i(t_p + \delta t/2)$ is calculated according to equation (3)

$$v_i(t_p + \delta t/2) = v_i(t_p - \delta t/2) + (f_i(t_p) + \lambda g_i^{(s)}(t_p))\delta t/m_i.$$

23. The method of Claim 16, further comprising calculating for each snap shot p a thermodynamic property $\Gamma(t_p)$, calculating a cumulated average thermodynamic property $\Gamma_c(t_p)$ according to equation (4): $\Gamma_c(t_p) = (1-x)\,\Gamma_c(t_p-1) + x\,\Gamma(t_p)$ where x is a number between 0 and 1.

24. A method of predicting an unknown folded structure of a polypeptide comprising:

generating a molecular dynamics trajectory according to the method of claim 16, wherein said molecular system comprises said polypeptide and said initial frame is defined by disposing said polypeptide in a random conformation; calculating a thermodynamic property along said trajectory; and extracting from said trajectory a selected frame associated with a predetermined criterion based on

said thermodynamic property and forming a predicted conformation by assigning to each atom in said polypeptide a corresponding position in said selected frame.

25. The method of Claim 20, wherein said molecular system is formed by said polypeptide immersed in a box of water molecules.

26. A method of determining a tertiary structure of a protein comprising generating a molecular dynamics simulation according to the method of Claim 16.

27. A method according to Claim 22, wherein determining said tertiary structure comprises processing data obtained through X-Ray crystallography or NMR.